Computer and Information Sciences
Materials Simulations

Two-Temperature Model of Radiation Damage

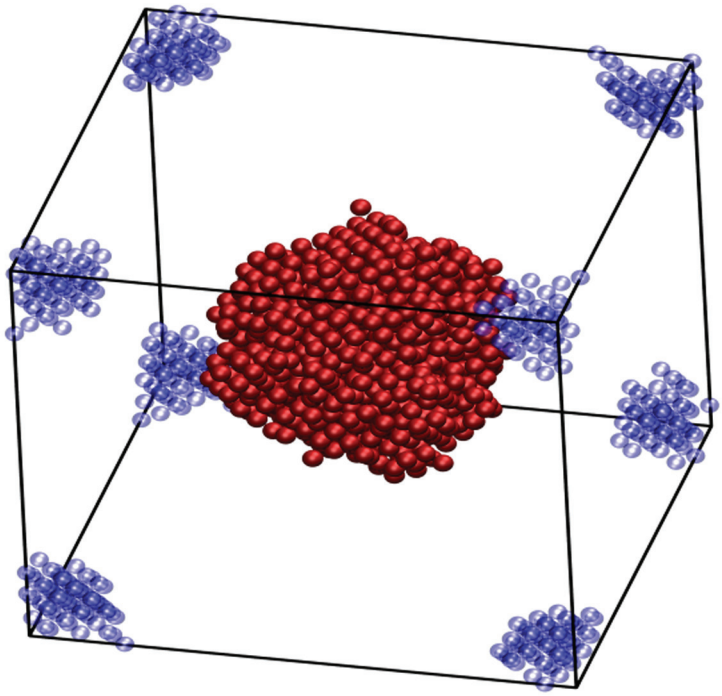

Figure 1: The initial state of the radiation-damaged system. The simulation box is the size of a 17×17×17 FCC unit cell system. The red liquid spot at the center initially consists of 1174 atoms. The 458 atoms that are tightly coupled to an infinite heat reservoir at a very low temperature are shown at the corners of the simulation cell (they form a sphere in periodic space). The 17,930 atoms that are neither defect atoms nor heat sink atoms are not shown.

Simulating radiation damage will provide more insights for the improvement of radiation-resistant circuitry

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Electronic circuits that are resistant to low or high dose radiation damage are vital to Sandia's missions in nuclear weapons and satellites. Advances in radiation hardening technology will require better understanding of the atomistic details of radiation damage processes. Molecular simulation is a powerful tool for exploring such atomistic processes, but current methods neglect essential effects of energized electrons. These effects can be included in classical molecular dynamics (MD) simulations by coupling the atom motions to a continuum representation of the electrons through a two-temperature model (TTM) [1-3], in which the electronic subsystem is represented with the heat equation solved on a grid to mimic the thermal response of the excited carrier electrons. The two subsystems are coupled through TTM-prescribed energy exchanges. Previous work has demonstrated TTM coupling by using an inhomogeneous and finite Langevin thermostat [3].

TTMs attempt to capture the interplay between electrons and atoms in a material during thermal transients such as radiation damage by modeling the electrons and the atoms as two separate systems, with two separate temperatures that are able to exchange energy through frictional forces applied to the atoms. In collaboration with the University of Michigan (involving a DOE Computational Science Graduate Fellow), Sandia has improved the simulations by introducing an energy-conserving version of the TTM to communicate energy between the electronic and atomic subsystems. This modification allows the inhomogeneous TTM to be used for longer and larger simulations, as well as for simulations of small energy phenomena, without introducing nonphysical energy fluctuations that may affect simulation results.

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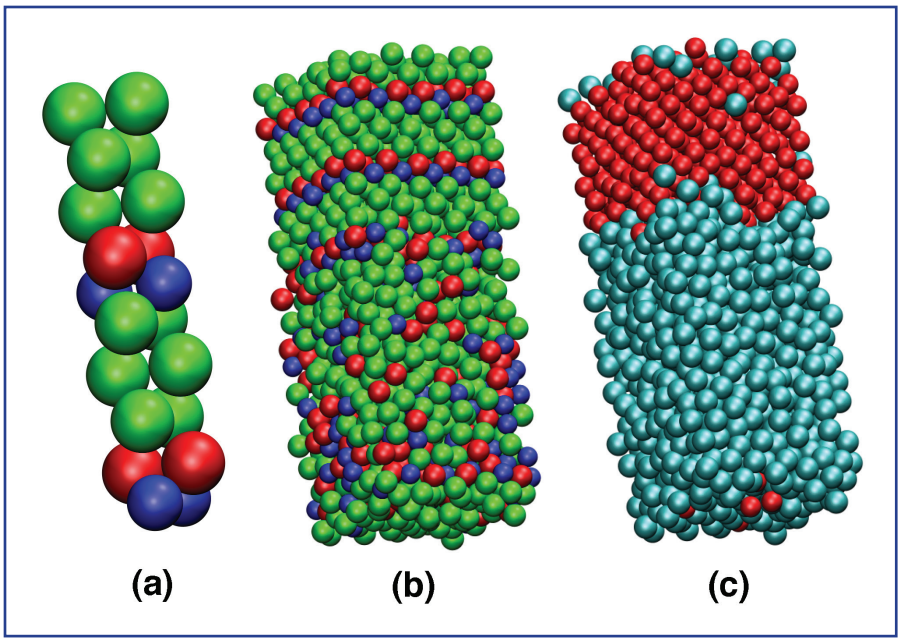

Figure 2: a) Two unit cells of the binary LJ system are shown. Species A is colored red in the AB CsCl phase and green in the A (FCC) phase. Species B is colored blue. Together, these two unit cells represent the smallest translatable unit for this crystal. (b) A two-thirds melted 5×5×6 crystal of binary LJ system. (c) The atoms of (b) have been re-labeled as crystalline (red) or non-crystalline (cyan). This figure was featured on the cover of the *Journal of Chemical Physics*, Vol. 131, Issue 7 (August 21st, 2009).

Significantly, the team was able to show that the previously published TTM+MD approach [3] leaks energy. The improved version was added to Sandia's massively parallel MD code, LAMMPS [4], and used for the simulations of radiation damage in single-component and binary Lennard-Jones (LJ) crystals [1].

The single-component face-centered-cubic (FCC) LJ crystals show remarkable resilience to radiation damage (Figure 1), whereas the binary glass-forming LJ crystal retained damage much more easily (Figure 2). For both of these LJ systems, a scan of TTM parameter space was performed to investigate how the electronic subsystem properties and its coupling with the atomic subsystem influenced material damage. A special shape-matching algorithm was used to identify damaged material.

In general, these models can be used to capture other high-energy events such as laser heating, sputtering, shock-induced melting, heterogeneous melting, and cascade simulations. Thus, Sandia will be able to perform increasingly improved simulations to the many critical processes that impact both materials and electronic components.

References

1. Phillips, C.L., and Crozier, P.S. (2009). An energy-conserving two-temperature model of radiation damage in single-component and binary Lennard-Jones crystals, *J. Chem. Phys.*, Vol. 131, Article No. 074701.
2. Greathouse, J.A., Crozier, P.S., Ismail, A.E., and Foiles, S.M. (2009). *The Effect of Electron-Ion Coupling on Radiation Damage Simulations of a Pyrochlore Waste Form*, SAND2009-6892. Sandia National Laboratories, Albuquerque, NM.
3. Duffy, D. M. and Rutherford, A. M. (2007). Including the effects of electronic stopping and electron-ion interactions in radiation damage simulations, *J. Phys.: Condens. Matter*, Vol. 19, Article No. 016207.
4. The TTM-MD module for LAMMPS is available for download as part of the LAMMPS MD package at http://lammps.sandia.gov. Specifically, see: http://lammps.sandia.gov/doc/fix_ttm.html

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